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Ab Initio Study of Deformation Influence on the Electronic Properties of Graphene Structures Containing One-Dimensional Topological Defects

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Abstract

© 2016, Springer Science+Business Media New York.The band structures of single and bilayer graphene with one-dimensional topological defects were calculated along the defect line, and appearance of the flat band near the Fermi level was observed. In addition, the influence of deformation (compression/expansion) on the flat band was studied. It was shown that compression across the grain boundary leads to disappearance of the flat band near the Fermi level, while the stretching along this direction does not significantly change the band structure. However, neither compression nor stretching along the grain boundary destroys the flat band.

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Keywords

Ab initio, Band structure, Defects, Flat band, Graphene